

Speakers

- > Prof TP Singh, All India Institute of Medical Sciences, New Delhi
- Prof N Srinivasan, Indian Institute of Science, Bengaluru
- > Prof R Sowdhamini, National Centre for Biological Sciences, Bengaluru
- > Dr Ashutosh Kumar, Indian Institute of Technology Bombay, Mumbai
- Dr Shashi Bhushan Pandit, Indian Institute of Science Education and Research, Mohali
- > Dr Ehesan Ali, Institute of Nano Science & Technology, Mohali
- > Dr Amit Nargotra, CSIR-Indian Institute of Integrative Medicine, Jammu
- > Dr Manoj Kumar, CSIR-IMTECH, Chandigarh
- > Dr Ashish, CSIR-IMTECH, Chandigarh
- > Dr Krishan Gopal, CSIR-IMTECH, Chandigarh
- > Dr Beena Krishnan, CSIR-IMTECH, Chandigarh
- > Dr Anshu Bhardwaj, CSIR-IMTECH, Chandigarh
- > Dr S Srikrishna, CSIR-IMTECH, Chandigarh
- Sh Chandershekhar Sharma, CSIR-IMTECH
- > Dr Balvinder Singh, CSIR-IMTECH, Chandigarh

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Computational Analysis of Protein Structures (CAPS)

A National Training Programme

9th to 13th December 2019

Schedule



Organized by:

Bioinformatics Centre (BIC), Institute of Microbial Technology, Chandigarh, India

Supported by Council of Scientific and Industrial Research and Department of Biotechnology, New Delhi

	9 th December, 2019	14:00	Demo and Hands on Session – Ehesan Ali
09:00	Registration	15:30	Теа
09:30	Introduction to Training Programme – B Singh	16:00	Demo and Hands on Session – Ehesan Ali
09:35	Welcome –Director, CSIR-IMTECH	20:00	Dinner
09:40	Bioinformatics Centre at IMTECH: Highlights and Introduction of		10 th December 2010
09:45	Speaker – S Srikrishna Protein structure to Bioinformatics to Drug Discovery– TP Singh	09:30	12th December, 2019 Quantitative structure–activity relationship (C models development using machine learning
10:30 11:00	High Tea Computational analysis of protein-protein interactions – R Sowdhamini	10:15	antiviral drug discover Talk - M Kumar Application of cheminformatics in drug discov
12:00	Revisiting India's pride: The Ramachandran map - all over again	11:00	Nargotra Tea
	– N Srinivasan	11:30	Protein Sequence Structure function Analysis
13:00 14:00	Lunch Bridging the islands of protein families in sequence space using	11.50	Noteworthy examples of Zn finger proteins by Srikrishna
4 4 4 5	artificial sequences – N Srinivasan	12:15	Demo and Hands on session – A Nargotra
14:45	Introduction to Linux/UNIX – C Sharma/A Yadav	13:00	Lunch
15:30 16:00	Tea Installation of Linux – Demo -Hands on Session – C Sharma/A	14:00	Tour to IMTECH facilities- Virtual Reality and Printing – Demo- S Srikrishna
00.00	Yadav	15:30	Теа
20:00	Dinner	16:00	Demo and Hands on Session – A Nargotra
	10 th December, 2019	20:00	Dinner
09:30	A Talk by K Gopal		4h
10:15	Demo and Hands on session – K Gopal		13 th December, 2019
11:00	Теа	09:30	Dynamic Hybrid Pharmacophore Approach for
11:30	Merging low resolution (SAXS) information with low confidence		Discovery of New Drugs - A Bhardwaj
	(MD or modeling) data to understand proteins - Ashish	10:30	Combining bioinformatics and experimental
12:15	Landscape of intra-chain domain-domain Interfaces – SB Pandit		approaches to understand "protein sequence
13:00	Lunch		function and disease" relationships - Beena
14:00	Demo and Hands on session – SB Pandit	11:15	Теа
16:00	Теа	11:45	Structure-Toxicity link of protein aggregates i
16:30	Demo and Hands on Session – Ashish		diseases - A Kumar
20:00	Dinner	13:00	Lunch
		14:30	Interactive Session
	11 th December, 2019	15:00	Valedictory Function
09:30	Computational mutagenesis reveals amino acids that play a role	15:30	Теа
00.00	in the entry of ion in active site of DHBPS: Mechanistic insights	Note:	

12th December, 2019 Quantitative structure-activity relationship (QSAR) models development using machine learning for antiviral drug discover Talk - M Kumar Application of cheminformatics in drug discovery-A Nargotra Теа Protein Sequence Structure function Analysis: Noteworthy examples of Zn finger proteins by S Srikrishna Demo and Hands on session - A Nargotra Lunch Tour to IMTECH facilities- Virtual Reality and 3D Printing – Demo- S Srikrishna Теа Demo and Hands on Session - A Nargotra Dinner 13th December, 2019 Dynamic Hybrid Pharmacophore Approach for Discovery of New Drugs - A Bhardwaj Combining bioinformatics and experimental approaches to understand "protein sequence to

- function and disease" relationships Beena Krishnan Теа Structure-Toxicity link of protein aggregates in human diseases - A Kumar Lunch Interactive Session
- Valedictory Function
- Tea

Note:

- Registration of training program will take place at reception area of IMTECH-Main building.
- Talks will be held in Crystal Room, GNR Protein Centre except the inaugural function. Demo-Hands-on Session will be in user lab, first floor, GNR protein Centre.
- Breakfast and dinner will be served in the Guest House for participants.
- Lunch will be served all days in the cafeteria, unless otherwise notified.

13:00 Lunch

Tea

from MD Simulations – B Singh

Demo and Hands on Session - B Singh

Bi-radical Perspective - Ehesan Ali

Modeling Protein Structures - Demo cum-Lecture- S Beriwal

In Silico Investigations of Antimalarial Activities of Artemisinin: A

10:15

11:00

11:30

12:15